Cumene

98-82-8 | DTXSID1021827

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.23 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.44e-01

Confidence level: 7.19e-01

Nearest Neighbors from the Training Set

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Furfural
Measured: 4.50
Predicted: 4.06

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2-Ethylhexyl acrylate
Measured: 3.42
Predicted: 3.32e-01

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Acetic acid, 2-nitrophenyl ester
Measured: 2.61
Predicted: 2.90e-03

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Dehydroacetic acid
Measured: 1.69
Predicted: 1.80e-03

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Linolenic acid
Measured: 3.61e-01
Predicted: 5.71e-07